SciApps - 10
Challenges and Opportunities for Scientific Applications:
learning to sustain the Petaflop with eyes on the Exaflop horizon.

This Workshop will bring together an interdisciplinary team of computational scientists to share experience, knowledge, and best practices on the implementation of a wide range of scientifically demanding and computationally paced applications on leading-edge high-performance scientific computer systems. Our goal for this workshop is to offer a cross discipline venue to facilitate interactions among current and potential leadership class computing users, explore opportunities to strengthen application development and obtain insight into near term and medium term application requirements and scientific mission goals. Access to DOE's Leadership Class Computing facilities is open to any academic, government, or industry research organization via the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program (http://DOEleadershipcomputing.org and http://www.sc.doe.gov/ascr/incite/).

When: August 3 – 6, 2010
Where: Oak Ridge National Laboratory, Building 5100 (JICS) Room 128

Agenda

August 3 2010

Time	Session	Speaker
8:00	Welcome and Purpose	Ricky Kendall and Doug Kothe
8:30	DOE Leadership Computing Overview	David Dean, DOE/ORNL
9:00	Future Directions of Computational Science	David Dean, DOE/ORNL
9:30	NSF Computing Overview	Irene Qualters, NSF
10:00	Break	
10:15	The INCITE Program	Julia White, ORNL
10:30	Architecture Overview	Steve Poole, ORNL
	Computational Science Software Ecosystem	
11:30	Programming Models	Bill Gropp, UIUC
12:15	Lunch: Scientific Visualization of the OLCF	Ross Toedte, ORNL
	Computational Science Software Ecosystem	
13:15	Operating Systems	Al Geist, ORNL
13:45	Libraries	Roger Pawlowski, Sandia
14:15	Requirements Gathering, Validation, and Synthesis	Hai Ah Nam, ORNL
14:45	What Software Engineering Practices Computational Scientists should know and use	Wayne Joubert, ORNL
15:30	Break	
15:45	The Joule Exercise: Importance and Impact	Rebecca Hartman-Baker, ORNL
16:15	The path to Exascale Computing	Buddy Bland, ORNL
16:45	Tour of the OLCF	NCCS staff
17:00	Adjourn for the Day	

August 4 2010

Time	Session	Speaker
8:00	Case Study: S3D	Ramanan Sankaran, ORNL
8:30	Requirements and science goals for sustained petascale Combustion Science	Guilhem Lacaze, Sandia
9:15	Future requirements and science goals for Combustion Science	Ray Grout, NREL
10:00	Break	
10:15	Case Study: Denovo	Tom Evans, ORNL
10:45	Requirements and science goals for sustained petascale Nuclear Energy	John Turner, ORNL
11:30	Future requirements and science goals for Nuclear Energy	Doug Kothe, ORNL
12:15	Lunch: UAO Overview	Ashley Barker, ORNL
1:30	Case Study: Chimera/Genesis	Bronson Messer, UT/ORNL
2:00	Requirements and science goals for sustained petascale Astrophysics	Paul Ricker, UIUC
2:45	Future requirements and science goals for Astrophysics	Christian Cardall, UT
3:30	Break	
3:45	Case Study: QASPR/Charon	Joe Castro, Sandia
4:15	Requirements and science goals for sustained petascale National Security	Rob Hoekstra, Sandia
5:00	Future requirements and science goals for National Security	Rob Hoekstra, Sandia
5:45	Adjourn	
6:00	Dinner:	Speaker TBD
7:30	Buses depart for hotel	

August 5 2010

Time	Session	Speaker
8:00	Case Study: WL-LSMS and DCA++	Markus Eisenbach, ORNL
8:30	Requirements and science goals for sustained petascale Materials and Nanoscience	Shiwei Zhang, William and Mary
9:15	Future requirements and science goals for Materials and Nanoscience	Thomas Schulthess, CSCS
10:00	Break	
10:15	Case Study: NWChem	Edo Apra, ORNL
10:45	Future requirements and science goals for Chemistry	Robert Harrison, ORNL
11:30	Lunch: NICS Overview	Christian Halloy, NICS
1:30	Case Study:GTC	Stephane Ethier, PPPL
2:00	Requirements and science goals for sustained petascale Fusion Simulation	CS Chang, NYU
2:45	Future requirements and science goals for Fusion Simulation	Bill Tang, PPPL
3:30	Break	

3:45	Case Study: Gromacs	Roland Schulz UT/ORNL
4:15	Requirements and science goals for sustained petascale Biophysics	Jeremy Smith, UT/ORNL
5:00	Future requirements and science goals for Biophysics	W. Michael Brown, ORNL
5:45	Adjourn	

August 6 2010

8:00	Case Study: MADNESS	Matt Reuter, Northwestern
8:30	Requirements and science goals for sustained petascale for the MADNESS framework	George Fann, ORNL
9:15	Future requirements and science goals for the MADNESS framework	Robert Harrison, UT/ORNL
10:00	Break	
10:15	Case Study: NUCOR	Hai Ah Nam, ORNL
10:45	Requirements and science goals for sustained petascale	James Vary, ISU
11:30	Future requirements and science goals for	Tom Luu, LLNL
12:15	Lunch: Application Performance Tools	Rich Graham, ORNL
1:30	Case Study: CCSM	Pat Worley, ORNL
2:00	Requirements and science goals for sustained petascale Climate Science	Trey White, NCAR
2:45	Future requirements and science goals for Climate Science	Jim Hack, ORNL
3:30	Break	
3:45	Workshop Roundtable Discussion	Doug Kothe
4:45	Wrap up	Ricky Kendall
5:00	Adjourn	